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0.21

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=> s hofmann, t?/au

L1 1518 HOFMANN, T?/AU

=> s ottinger, h?/au

L2 252 OTTINGER, H?/AU

h eb c g cg b cg

eb

=> s frank, o?/au
 L3 743 FRANK, O?/AU

=> s soldo, t?/au
 L4 19 SOLDO, T?/AU

=> s blank, i?/au
 L5 397 BLANK, I?/AU

=> s villard, r?/au
 L6 28 VILLARD, R?/AU

=> s robert, f?/au
 L7 1376 ROBERT, F?/AU

=> d his

(FILE 'HOME' ENTERED AT 18:32:48 ON 28 NOV 2004)

FILE 'MEDLINE, BIOSIS, CAPLUS, EMBASE' ENTERED AT 18:33:00 ON 28 NOV 2004

L1 1518 S HOFMANN, T?/AU
 L2 252 S OTTINGER, H?/AU
 L3 743 S FRANK, O?/AU
 L4 19 S SOLDO, T?/AU
 L5 397 S BLANK, I?/AU
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 L7 1376 S ROBERT, F?/AU

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 L8 1 L1 AND L2 AND L3 AND L4 AND L5 AND L6 AND L7

=> d l8, ibib abs, 1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION-NUMBER: 2003:201514 CAPLUS
 DOCUMENT NUMBER: 138:221853
 TITLE: Preparation of pyridinium-betaine compounds as taste enhancers
 INVENTOR(S): Hofmann, Thomas; Ottinger, Harald; Frank, Oliver; Soldo, Tomislav; Blank, Imre; Villard, Renaud; Robert, Fabien
 PATENT ASSIGNEE(S): Societe des Produits Nestle S.A., Switz.
 SOURCE: Eur. Pat. Appl., 17 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1291342	A1	20030312	EP 2001-121349	20010906
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
WO 2003022817	A1	20030320	WO 2002-EP10368	20020905
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
 TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
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 PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
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EP 1427703 A1 20040616 EP 2002-797989 20020905

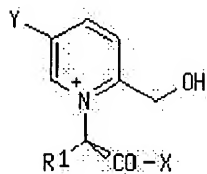
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US 2004171648 A1 20040902 US 2004-792369 20040302

PRIORITY APPLN. INFO.: EP 2001-121349 A 20010906
 WO 2002-EP10368 W 20020905

OTHER SOURCE(S): MARPAT 138:221853

GI



AB The invention concerns pyridinium-betaine compds. I (R1 is the side chain of a primary L-amino acid; X, Y are OH or O-), in which the counter ion is sodium, potassium, ammonium, calcium, magnesium, chloride, nitrate, carbonate, sulfate, phosphate, etc., for use as taste enhancers. Thus, treatment of 5-(hydroxymethyl)-2-furancarboxaldehyde with L-alanine in H2O/EtOH (1:1; pH 9.4) at reflux for 3 days afforded (S)-alapyridaine (I; R1 = Me, X = O-, Y = OH), which has a sweet taste.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 L3 743 S FRANK, O?/AU
 L4 19 S SOLDI, T?/AU
 L5 397 S BLANK, I?/AU
 L6 28 S VILLARD, R?/AU
 L7 1376 S ROBERT, F?/AU
 L8 1 S L1 AND L2 AND L3 AND L4 AND L5 AND L6 AND L7

=> s l1 and l3

L9 52 L1 AND L3

=> s l1 and l3 and l2

L10 10 L1 AND L3 AND L2

=> s l1 and l3 and l2 and l4 and l5

L11 3 L1 AND L3 AND L2 AND L4 AND L5

=> d his

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 L5 397 S BLANK, I?/AU
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 L7 1376 S ROBERT, F?/AU
 L8 1 S L1 AND L2 AND L3 AND L4 AND L5 AND L6 AND L7
 L9 52 S L1 AND L3
 L10 10 S L1 AND L3 AND L2
 L11 3 S L1 AND L3 AND L2 AND L4 AND L5

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L12 2 L11 NOT L8

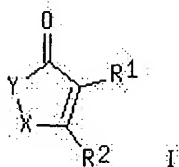
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L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

Full Text	References
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ACCESSION NUMBER: 2004:219832 CAPLUS
 DOCUMENT NUMBER: 140:252679
 TITLE: Consumable product including consumable component and
 alpha-keto enamine derivatives
 INVENTOR(S): Hofmann, Thomas; Ottinger, Harald; Frank,
 Oliver; Soldi, Tomislav; Cerny, Christoph; Robert,
 Fabien; Blank, Imre
 PATENT ASSIGNEE(S): Germany
 SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S.
 Pat. Appl. 2002 22,039.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004052828	A1	20040318	US 2003-448306	20030530
US 2002022039	A1	20020221	US 2001-863970	20010523
US 6592884	B2	20030715		
PRIORITY APPLN. INFO.:			EP 2000-110886	A 20000523
			US 2001-863970	A2 20010523
OTHER SOURCE(S):			MARPAT 140:252679	
GI				



AB A consumable product that includes a consumable component and a cooling component present in an amt. sufficient to provide a cooling sensation to a consumer, which cooling component includes one or more compds. each having the general formula (I): wherein R1 is selected from the group consisting of N-Pyrrolidinyl, N-Pyridinyl, N-(aminodiethyl), N-(2-carboxy-pyrrolidinyl), piperidinyl, or N-(2-Methoxycarbonyl-pyrrolidinyl); R2 is selected from the group consisting of H or Me; X is selected from the group consisting of methylene, ethylidene, 1-Propylidene, or oxy radical; and Y is selected from the group consisting of methylene, ethylidene, 1-propylidene, oxy radical, ethan-1,2-diyl, ethen-1,2-diyl, propan-1,2-diyl, or ethan-1-oxy-1-yl, provided that when R1 is N-pyrrolidinyl, X is methylene, and Y is ethylidene then R2 cannot be H, and provided that when R1 is N-pyrrolidinyl, and X and Y are each methylene, then R2 cannot be Me. In particular, the consumable product can be a food product, perfume, cosmetic, or pharmaceutical.

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

Full Text Cite
References

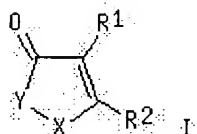
ACCESSION NUMBER: 2001:864700 CAPLUS
DOCUMENT NUMBER: 136:5066
TITLE: Use of alpha-keto enamine derivatives as ingredients
INVENTOR(S): Hofmann, Thomas; Ottinger, Harald; Frank, Oliver; Soldo, Tomislav; Cerny, Christoph; Robert, Fabien; Blank, Imre
PATENT ASSIGNEE(S): Societe des Produits Nestle S.A., Switz.
SOURCE: Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1157617	A2	20011128	EP 2001-111959	20010521
EP 1157617	A3	20020911		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 2001004188	A	20021122	ZA 2001-4188	20010522
CA 2348301	AA	20011123	CA 2001-2348301	20010523
CN 1334031	A	20020206	CN 2001-124817	20010523
BR 2001002083	A	20020319	BR 2001-2083	20010523
JP 2002084990	A2	20020326	JP 2001-153799	20010523
NZ 511903	A	20021220	NZ 2001-511903	20010523
			EP 2000-110886	A 20000523

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 136:5066

GI



AB The present invention concerns the use of a compd. of general formula I alone or in combination, as an ingredient for food, cosmetic, pharmaceutical and perfume compns., wherein R1 is N-pyrrolidinyl, R2 is

Me, X is Ethylidene and Y is an Oxy radical.

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 L5 397 S BLANK, I?/AU
 L6 28 S VILLARD, R?/AU
 L7 1376 S ROBERT, F?/AU
 L8 1 S L1 AND L2 AND L3 AND L4 AND L5 AND L6 AND L7
 L9 52 S L1 AND L3
 L10 10 S L1 AND L3 AND L2
 L11 3 S L1 AND L3 AND L2 AND L4 AND L5
 L12 2 S L11 NOT L8

=> s l6 and l4 and l5

L13 4 L6 AND L4 AND L5

=> s l13 not l12

L14 4 L13 NOT L12

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L15 3 L14 NOT L8

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L15 ANSWER 1 OF 3 MEDLINE on STN

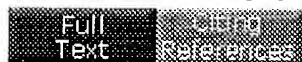
Full Text Reference

ACCESSION NUMBER: 2003335953 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 12822944
 TITLE: Racemic and enantiopure synthesis and physicochemical characterization of the novel taste enhancer N-(1-carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol inner salt.
 AUTHOR: Villard Renaud; Robert Fabien; Blank Imre; Bernardinelli Gerald; Soldo Tomislav; Hofmann Thomas
 CORPORATE SOURCE: Nestle Research Center, Vers-chez-les-Blanc, 1000 Lausanne 26, Switzerland.
 SOURCE: Journal of agricultural and food chemistry, (2003 Jul 2) 51 (14) 4040-5.
 Journal code: 0374755. ISSN: 0021-8561.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200308
 ENTRY DATE: Entered STN: 20030719
 Last Updated on STN: 20030821
 Entered Medline: 20030820

AB Convenient syntheses were developed to obtain on a multigram scale the novel taste enhancer N-(1-carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol 1, called alapyridaine, as a racemic mixture and as pure (+)-(S) and (-)-(R) enantiomers, respectively. 5-(Hydroxymethyl)-2-furaldehyde was

used as key intermediate and was reacted with L-alanine under alkaline conditions to obtain racemic 1. Alternatively, reductive amination of 5-(hydroxymethyl)-2-furaldehyde with Raney-Ni/hydrogen and L- or D-alanine followed by mild oxidation led to (+)-(S)-1 and (-)-(R)-1, respectively. Racemization was promoted under alkaline and boiling conditions via a carbanion, the formation of which was facilitated by the electron-withdrawing effect of the iminium cation and the resonance-stabilizing capacity of the pyridinium moiety. Under these conditions, 1 was obtained in a 1:1 mixture of the phenol (1) and phenolate (1-H) forms as shown by X-ray diffraction. Racemic 1 formed monoclinic crystals of high molecular organization in which the phenol-type (RS)-1, the phenolate-type (RS)-1-H, sodium cations, and ethanol molecules are present. The crystal structure of [Na(1)(1-H).(C(2)H(6)O)] shows one-dimensional $\mu(2)$ -bridging-oxygen polymers stabilized by a three-dimensional network of ionic, hydrogen bond, and pi-stacking interactions with channels occupied by solvent molecules.

L15 ANSWER 2 OF 3 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on STN



ACCESSION NUMBER: 2003:387310 BIOSIS
 DOCUMENT NUMBER: PREV200300387310
 TITLE: Racemic and enantiopure synthesis and physicochemical characterization of the novel taste enhancer N-(1-Carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol inner salt.
 AUTHOR(S): Villard, Renaud; Robert, Fabien; Blank, Imre [Reprint Author]; Bernardinelli, Gerald; Soldo, Tomislav; Hofmann, Thomas
 CORPORATE SOURCE: Nestle Research Center, Vers-chez-les-Blanc, 1000, P.O. Box 44, Lausanne, 26, Switzerland
imre.blank@rdls.nestle.com
 SOURCE: Journal of Agricultural and Food Chemistry, (July 2 2003) Vol. 51, No. 14, pp. 4040-4045. print.
 CODEN: JAFCAU. ISSN: 0021-8561.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 20 Aug 2003
 Last Updated on STN: 18 Sep 2003

AB Convenient syntheses were developed to obtain on a multigram scale the novel taste enhancer N-(1-carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol 1, called alapyridaine, as a racemic mixture and as pure (+)-(S) and (-)-(R) enantiomers, respectively. 5-(Hydroxymethyl)-2-furaldehyde was used as key intermediate and was reacted with L-alanine under alkaline conditions to obtain racemic 1. Alternatively, reductive amination of 5-(hydroxymethyl)-2-furaldehyde with Raney-Ni/hydrogen and L- or D-alanine followed by mild oxidation led to (+)-(S)-1 and (-)-(R)-1, respectively. Racemization was promoted under alkaline and boiling conditions via a carbanion, the formation of which was facilitated by the electron-withdrawing effect of the iminium cation and the resonance-stabilizing capacity of the pyridinium moiety. Under these conditions, 1 was obtained in a 1:1 mixture of the phenol (1) and phenolate (1-H) forms as shown by X-ray diffraction. Racemic 1 formed monoclinic crystals of high molecular organization in which the phenol-type (RS)-1, the phenolate-type (RS)-1-H, sodium cations, and ethanol molecules are present. The crystal structure of (Na(1)(1-H)cntdot(C2H6O)) shows one-dimensional μ_2 -bridging-oxygen polymers stabilized by a three-dimensional network of ionic, hydrogen bond, and pi-stacking interactions with channels occupied by solvent

molecules.

L15 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

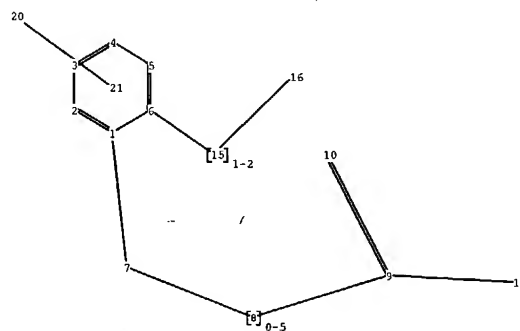
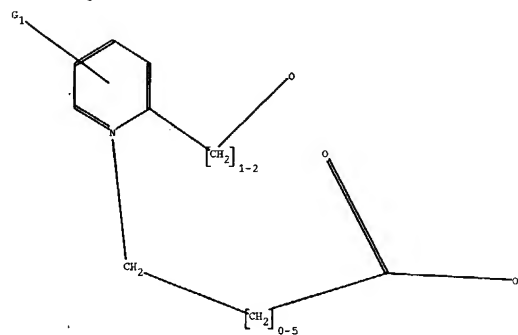
Full Text Citations

ACCESSION NUMBER: 2003:421335 CAPLUS
DOCUMENT NUMBER: 139:133445
TITLE: Racemic and Enantiopure Synthesis and Physicochemical Characterization of the Novel Taste Enhancer N-(1-Carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol Inner Salt
AUTHOR(S): Villard, Renaud; Robert, Fabien; Blank, Imre; Bernardinelli, Gerald; Soldo, Tomislav; Hofmann, Thomas
CORPORATE SOURCE: Nestle Research Center, Lausanne, 1000, Switz.
SOURCE: Journal of Agricultural and Food Chemistry (2003), 51(14), 4040-4045
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133445

AB Convenient syntheses were developed to obtain on a multigram scale the novel taste enhancer N-(1-carboxyethyl)-3-hydroxy-6-(hydroxymethyl)pyridinium (I), called alapyridaine, as a racemic mixt. and as pure (+)-(S) and (-)-(R) enantiomers, resp. 5-(Hydroxymethyl)-2-furaldehyde was used as key intermediate and was reacted with L-alanine under alk. conditions to obtain racemic I. Alternatively, reductive amination of 5-(hydroxymethyl)-2-furaldehyde with Raney-Ni/hydrogen and L- or D-alanine followed by mild oxidn. led to (+)-(S)-I and (-)-(R)-I, resp. Racemization was promoted under alk. and boiling conditions via a carbanion, the formation of which was facilitated by the electron-withdrawing effect of the iminium cation and the resonance-stabilizing capacity of the pyridinium moiety. Under these conditions, I was obtained in a 1:1 mixt. of the phenol I and phenolate (I-H) forms as shown by X-ray diffraction. Racemic I formed monoclinic crystals of high mol. organization in which the phenol-type (RS)-I, the phenolate-type (RS)-I-H, sodium cations, and ethanol mols. are present. The crystal structure of [Na(I)(I-H)·(C₂H₆O)] shows one-dimensional μ 2-bridging-oxygen polymers stabilized by a three-dimensional network of ionic, hydrogen bond, and π -stacking interactions with channels occupied by solvent mols.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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chain nodes :
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 1 2 3 4 5 6
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 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
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 exact bonds :
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Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 15:CLASS 16:CLASS 20:CLASS 21:CLASS

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 NEWS 6 SEP 27 STANDARDS will no longer be available on STN
 NEWS 7 SEP 27 SWETSCAN will no longer be available on STN
 NEWS 8 OCT 28 KOREAPAT now available on STN
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 and SOLIDSTATE reloads

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004

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FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

DICTIONARY FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DICTIONARY FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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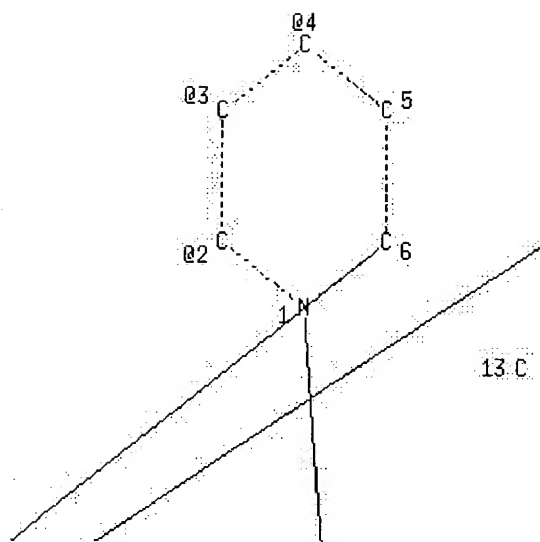
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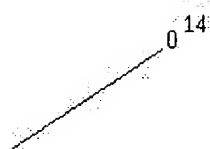
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0 17 S 18

G1 016



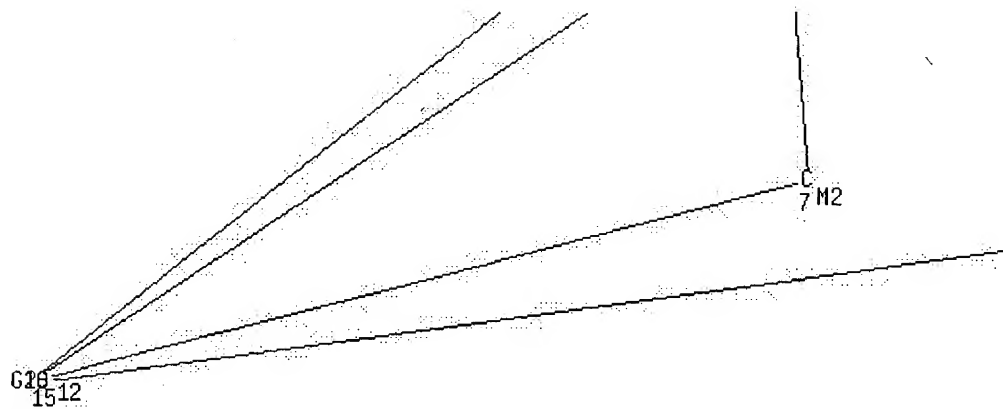
Page 1-A



M2



Page 1-B



Page 2-A

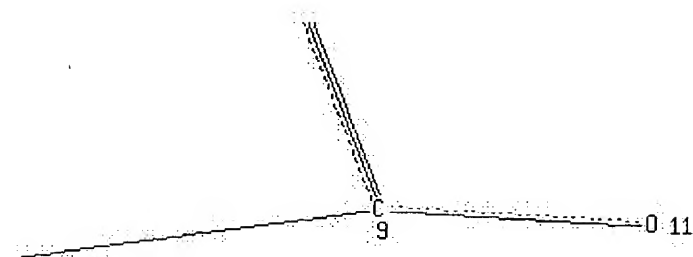
h

eb c

g cg b

cg

eb



8.C M2

Page 2-B

VAR G1=17/18

REP G19=(1-2) 13-6 13-14

REP G20=(0-5) 8-7 8-9

VPA 16-2/3/4 S

NODE ATTRIBUTES:

HCOUNT	IS M2	AT	7
HCOUNT	IS M2	AT	8
HCOUNT	IS M2	AT	13
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS C	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 8 9 10 11 13 14 17 18

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 18:17:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 10 TO ITERATE

100.0% PROCESSED 10 ITERATIONS

SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 11 TO 389

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> \$ 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:17:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 156 TO ITERATE

100.0% PROCESSED 156 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> file medline, biosis, caplus, embase
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.94	158.57

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FILE 'BIOSIS' ENTERED AT 18:18:11 ON 28 NOV 2004
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=>

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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 "Ask CAS" for self-help around the clock
 NEWS 3 SEP 01 INPADOC: New family current-awareness alert (SDI) available
 NEWS 4 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
 STN Express with Discover!
 NEWS 5 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
 NEWS 6 SEP 27 STANDARDS will no longer be available on STN
 NEWS 7 SEP 27 SWETSCAN will no longer be available on STN
 NEWS 8 OCT 28 KOREAPAT now available on STN
 NEWS 9 NOV 18 Current-awareness alerts, saved answer sets, and current
 search transcripts to be affected by CERAB, COMPUAB, ELCOM,
 and SOLIDSTATE reloads

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004

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 specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 18:13:37 ON 28 NOV 2004

=> file req		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:13:43 ON 28 NOV 2004

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STRUCTURE FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

DICTIONARY FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

0.42 0.63

FILE 'REGISTRY' ENTERED AT 18:13:58 ON 28 NOV 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

DICTIONARY FILE UPDATES: 26 NOV 2004 HIGHEST RN 789461-15-0

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

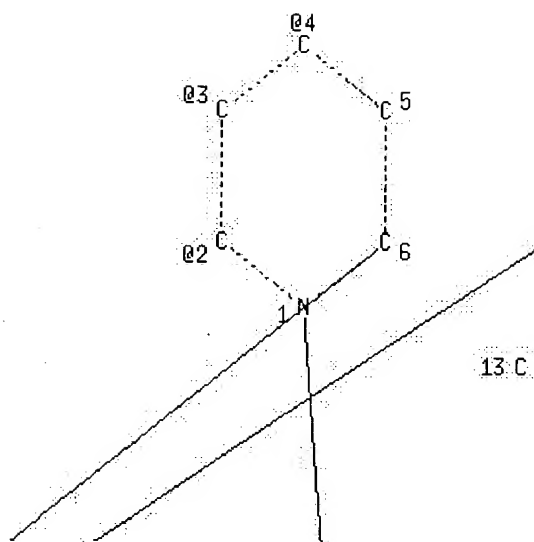
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L1 HAS NO ANSWERS

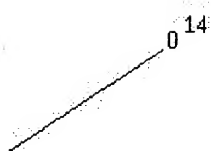
L1 STR

0 17 S 18

G1 016



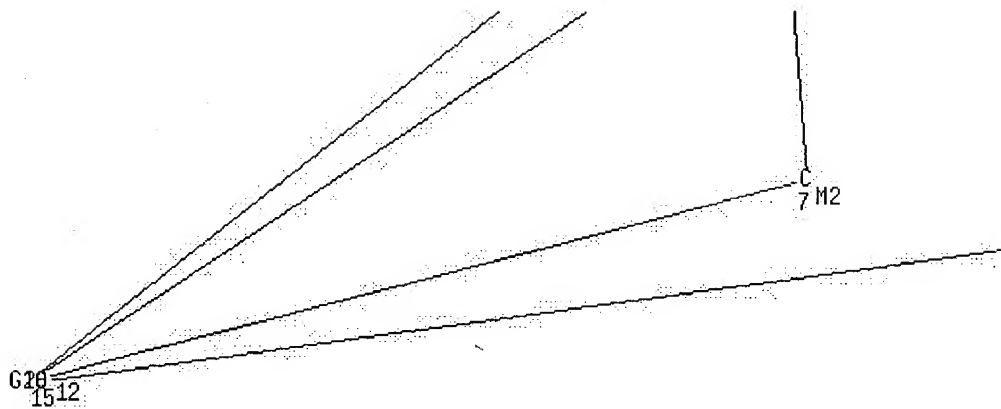
Page 1-A



M2



Page 1-B



Page 2-A

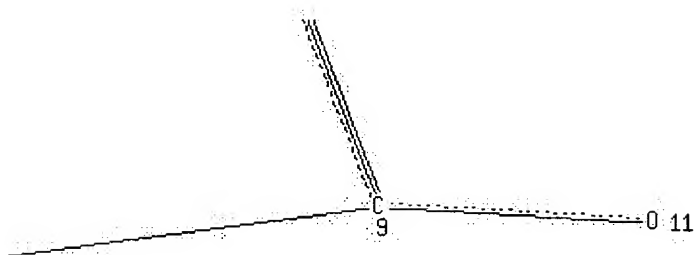
h

eb c

g cg b

cg

eb



8 CM2

Page 2-B

VAR G1=17/18

REP G19=(1-2) 13-6 13-14

REP G20=(0-5) 8-7 8-9

VPA 16-2/3/4 S

NODE ATTRIBUTES:

HCOUNT	IS M2	AT	7
HCOUNT	IS M2	AT	8
HCOUNT	IS M2	AT	13
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS C	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16

DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 7 8 9 10 11 13 14 17 18
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

=> s 1.1

SAMPLE SEARCH INITIATED 18:17:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 10 TO ITERATE

100.0% PROCESSED 10 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 11 TO 389

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s ll full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:17:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 156 TO ITERATE

100.0% PROCESSED 156 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> file medline, biosis, caplus, embase
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
157.94	158.57

FULL ESTIMATED COST

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=> s ll and ol, s?/au

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> d his

(FILE 'HOME' ENTERED AT 18:13:37 ON 28 NOV 2004)

FILE 'REGISTRY' ENTERED AT 18:13:43 ON 28 NOV 2004

FILE 'REGISTRY' ENTERED AT 18:13:58 ON 28 NOV 2004

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 FULL

FILE 'MEDLINE, BIOSIS, CAPLUS, EMBASE' ENTERED AT 18:18:11 ON 28 NOV 2004

=> s ol, s?/au

L4 1699 OL, S?/AU

=> s suzuki, n?/au

L5 14156 SUZUKI, N?/AU

=> s aso, k?/au

L6 1317 ASO, K?/AU

=> s banno, y?/au

L7 788 BANNO, Y?/AU

=> d his

(FILE 'HOME' ENTERED AT 18:13:37 ON 28 NOV 2004)

FILE 'REGISTRY' ENTERED AT 18:13:43 ON 28 NOV 2004

FILE 'REGISTRY' ENTERED AT 18:13:58 ON 28 NOV 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

FILE 'MEDLINE, BIOSIS, CAPLUS, EMBASE' ENTERED AT 18:18:11 ON 28 NOV 2004

L4 1699 S OL, S?/AU

L5 14156 S SUZUKI, N?/AU

L6 1317 S ASO, K?/AU

L7 788 S BANNO, Y?/AU

=> s l4 and l5

L8 0 L4 AND L5

=> s l4 and l6 and l7

L9 0 L4 AND L6 AND L7

=> s l7 and l6

L10 1 L7 AND L6

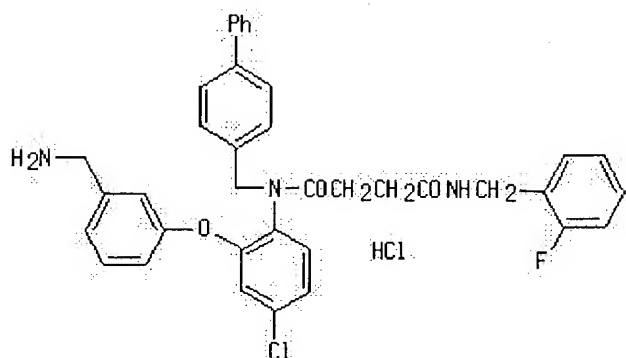
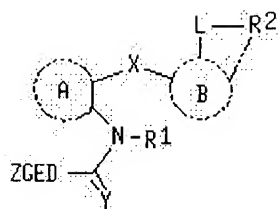
=> d l10, chib abs, 1

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

EBING
REFERENCES

2000:277959 Document No. 132:321662 Preparation of aromatic amine derivatives and agents containing the same. Oi, Satoru; Suzuki, Nobuhiro; Aso, Kazuyoshi; Banno, Yoshihiro (Takeda Chemical Industries, Ltd., Japan). PCT Int. Appl. WO 2000023420 A1 20000427, 309 pp. DESIGNATED STATES: W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1999-JP5755 19991019. PRIORITY: JP 1998-298940 19981020.

GI



AB Title compds. [I; wherein A is an optionally substituted arom. ring; B is an optionally substituted cyclic hydrocarbon oxy group; Z is an optionally substituted cyclic hydrocarbon group; R1 is hydrogen, optionally substituted hydrocarbyl, an optionally substituted heterocyclic group, or acyl; R2 is optionally substituted amino; D is a free valency or a divalent group; E is CO, CON(Ra), COO, N(Ra)CON(Rb), N(Ra)SO2, N(Ra), O, S, SO, SO2; G is a free valency or a divalent group; L is a free valency, an optionally substituted divalent hydrocarbon group which may be interrupted by O or S, or the like; X is oxygen, optionally oxidized sulfur, optionally substituted nitrogen, or an optionally substituted divalent hydrocarbon group; Y is two hydrogen atoms, oxygen, or sulfur; and the dotted line indicates that R2 and an atom on ring B may together form a ring] and salts are prepd. and tested as somatostatin receptor regulators. Thus, the title compd. II was prepd. in treatment or prevention of diabetes and obesity.

=> d his

(FILE 'HOME' ENTERED AT 18:13:37 ON 28 NOV 2004)

FILE 'REGISTRY' ENTERED AT 18:13:43 ON 28 NOV 2004

FILE 'REGISTRY' ENTERED AT 18:13:58 ON 28 NOV 2004

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 FULL

FILE 'MEDLINE, BIOSIS, CAPLUS, EMBASE' ENTERED AT 18:18:11 ON 28 NOV 2004

L4 1699 S OL, S?/AU
L5 14156 S SUZUKI, N?/AU
L6 1317 S ASO, K?/AU
L7 788 S BANNO, Y?/AU
L8 0 S L4 AND L5
L9 0 S L4 AND L6 AND L7
L10 1 S L7 AND L6

=> s 15 and 17

L11 1 L5 AND L7
 => s 111 not 110
 L12 0 L11 NOT L10

=> s 14 and 17
 L13 0 L4 AND L7

=> s 15 and 16
 L14 2 L5 AND L6

=> s 114 not 111
 L15 1 L14 NOT L11

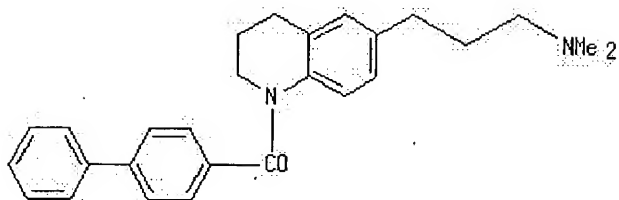
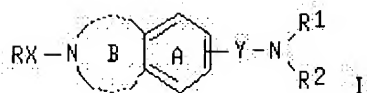
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L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

ACCESSION NUMBER: 2001:851111 CAPLUS
 DOCUMENT NUMBER: 136:5926
 TITLE: Preparation of benzoaromatic derivatives as melanin
 concentrating hormone antagonists
 INVENTOR(S): Ishihara, Yuji; Terauchi, Jun; Suzuki, Nobuhiro;
 Takekawa, Shiro; Aso, Kazuyoshi
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
 SOURCE: PCT Int. Appl., 285 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001087834	A1	20011122	WO 2001-JP4015	20010515
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001332407	A2	20011130	JP 2000-148674	20000516
JP 2002371059	A2	20021226	JP 2001-145691	20010515
EP 1283199	A1	20030212	EP 2001-930132	20010515
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003158177	A1	20030821	US 2002-276288	20021112
PRIORITY APPLN. INFO.:			JP 2000-148647	A 20000516
			JP 2001-116219	A 20010413
			JP 2000-148674	A 20000516
			WO 2001-JP4015	W 20010515
OTHER SOURCE(S):	MARPAT	136:5926		
GI				



AB Title compds. [I; R = H, halo, cyclic; X = bond, spacer contg. a chain with one to six atoms; Y = spacer with one to six atoms; A = benzene; B = 5-9 membered nitrogen contg. nonarom. heterocycle; R1 = H, hydrocarbon, heterocycle; R2 = H, hydrocarbon, heterocycle; R1R2 = nitrogen contg. heterocycle; YR2 = nitrogenous heterocycle], melanin-concg. hormone antagonist, which contains a compd. represented by the formula or a salt thereof are prepd. useful as prevention or remedy for adiposity, diabetes, or high blood pressure. Thus, the title compd. II was prepd. and biol. tested.

REFERENCE COUNT: 531 THERE ARE 531 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>